

## DETECTION OF INTERSTELLAR CYANOFORMALDEHYDE (CNCHO)

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### ABSTRACT

Cyanoformaldehyde (CNCHO) has been detected toward the star-forming region Sagittarius B2(N) with the 100 m Green Bank Telescope (GBT) by means of four *P*-branch rotational transitions in emission, the 7(0, 7)–6(1, 6) at 8.6 GHz, the 8(0, 8)–7(1, 7) at 19.4 GHz, the 9(0, 9)–8(1, 8) at 30.3 GHz, and the 10(0, 10)–9(1, 9) at 41.3 GHz, and one *P*-branch transition in absorption, the 5(1, 5)–6(0, 6) at 2.1 GHz. The five *b*-type transitions have favorable transition line strengths ( $S_{ij}\mu^2 > 10 D^2$ ) and occur in spectral regions that have little possibility of confusion with other molecular species. The transition line strengths and energy levels involved in the four cyanoformaldehyde transitions in emission are similar; however, transitions with larger beam sizes give systematically higher column densities, suggesting that CNCHO is spatially extended and not concentrated toward the Sgr B2(N-LMH) position. Moreover, with a GBT beamwidth of  $\sim 350'$ , the 5(1, 5)–6(0, 6) transition of CNCHO was detected in absorption, confirming the widespread spatial extent of this molecule. We suggest that cyanoformaldehyde is likely formed in a neutral-radical reaction of two other interstellar molecules known for widespread spatial distributions: formaldehyde ( $H_2CO$ ) and the cyanide (CN) radical.

*Subject headings:* ISM: abundances — ISM: clouds — ISM: individual (Sagittarius B2(N-LMH)) — ISM: molecules — radio lines: ISM

### 1. INTRODUCTION

Cyanoformaldehyde (CNCHO, aka formyl cyanide), shown schematically in Figure 1, is a planar asymmetric top molecule composed of two functional groups (i.e., the aldehyde and cyano groups) that are among the ones most commonly found in the interstellar medium. For example, CN was one of the very first molecules detected in interstellar space (McKellar 1940) and formaldehyde ( $H_2CO$ ) was the first organic, polyatomic molecule found in space (Snyder et al. 1969). Both  $H_2CO$  and CN are very common interstellar species and are found to be spatially widespread in interstellar clouds. Since CNCHO represents the simplest combination of the aldehyde and cyano functional groups possible, it would have been a prime candidate for an interstellar search. However, in the early stages of molecular spectral line astronomy CNCHO was believed to be an unstable species that would quickly undergo unimolecular decomposition into products of HCN and CO (e.g., Judge et al. 1986; Clouthier & Moule 1987).

The first rotational spectrum of CNCHO (millimeter wave) was reported in 1988 when it, along with propene, HCN, and CO, were formed via the flash vacuum thermolysis of allyloxycetonitrile (Bogey et al. 1988). Under these impure conditions, CNCHO exhibited a relatively short half-life of 29 minutes. From this work and a subsequent study (Bogey et al. 1995), rotational and distortion constants were determined for the CNCHO molecule. When CNCHO was finally created and studied (via FTIR) in its pure form (Lewis-Bevan et al. 1992), it was found to be

a stable species which could be frozen (77 K) and revaporized to room temperature without forming a polymeric material. Unimolecular decomposition was not observed. This same study showed that gas phase CNCHO is highly reactive with  $H_2O$ , forming products  $HCOOH$  and  $HCN$ . The latter three molecules are all found abundant in the interstellar medium. The activation energy barrier for CNCHO to decompose into CO and HCN is estimated to be  $68.74 \text{ kcal mol}^{-1}$  ( $\sim 16,700 \text{ K}$ ) from theoretical calculations (Lewis-Bevan et al. 1992). Therefore, once produced in the gas-phase interstellar medium, CNCHO should be stable and survive in low-density interstellar environments when shielded from the general stellar and Galactic radiation fields.

Several searches with three different telescopes for favorable millimeter-wavelength transitions of CNCHO have been reported but no transitions were detected (Woolf 2006; Gerin et al. 1989). These previous observational results suggested that a sensitive search for interstellar CNCHO be conducted at centimeter wavelengths where spectral line confusion is much less than at millimeter wavelengths. Herein we report the first successful search for interstellar CNCHO with the GBT 100 m telescope.

### 2. OBSERVATIONS AND RESULTS

Spectral line observations of cyanoformaldehyde were conducted with the NRAO<sup>8</sup> 100 m Robert C. Byrd Green Bank Telescope (GBT) on 2005 April 1 and November 12 (K band); 2005 September 6–19, November 10 (X band); 2007 November 7 (Ka band); 2007 November 9–10 (S band); and 2007 December 29 (Q band). The GBT spectrometer was configured to provide four intermediate frequency (IF) bandwidths at a time in two polarizations through the use of offset oscillators in the IF. Table 1 lists the cyanoformaldehyde rotational transition quantum numbers, the calculated transition center rest frequency, the transition line strength ( $S$ ), the lower energy level ( $E_l$ ), the telescope beamwidth ( $\theta_B$ ), and the telescope beam efficiency ( $\eta_B$ ) in the first six columns. The S-band, X-band, K-band, Ka-band, and Q-band receivers used

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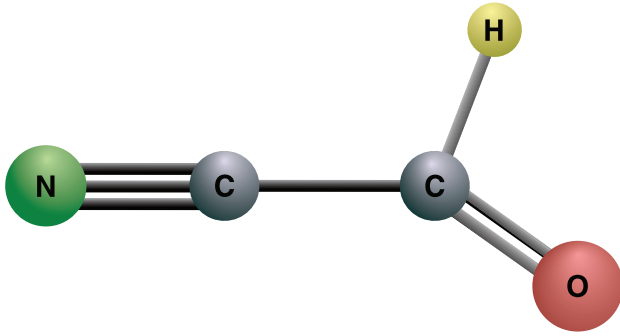


FIG. 1.—Schematic diagram showing the planar structure of CNCHO. For bond lengths and angles based on ab initio calculations, see Fig. 2 of Goddard (1986).

have frequency ranges covering 2–4 GHz, 8–10.1 GHz, 18–22.5 GHz, 26–40 GHz, and 40–48 GHz, respectively. The GBT spectrometer was configured in its 8 IF, 200 MHz, 3 level mode which provides observing of four 200 MHz frequency bands at a time in two polarizations through the use of offset oscillators in the IF. This mode affords 24.4 kHz channel separation. Antenna temperatures are on the  $T_A^*$  scale (Ulich & Haas 1976) with estimated 20% uncertainties. The Sgr B2(N-LMH) J2000.0 pointing position employed was  $\alpha = 17^{\text{h}}47^{\text{m}}19.8^{\text{s}}$ ,  $\delta = -28^{\circ}22'17''$ , and an LSR source velocity of  $+64 \text{ km s}^{-1}$  was assumed. Data were taken in the OFF-ON position-switching mode, with the OFF position  $60'$  east in azimuth with respect to the ON source position. For further observational details, see Hollis et al. (2004a). Pointing and focus corrections were adjusted typically every 2 hours or less using the calibrators 1626–298, 1733–130, or 1700–2610. The two polarization outputs and data taken over multiple days were averaged in the final data reduction process to improve the signal-to-noise ratio. Note, however, that the Ka-band receiver was limited to only one polarization during these observations.

Table 1 summarizes the cyanoformaldehyde emission and absorption features searched for toward Sgr B2(N) in terms of LSR velocities and corresponding Gaussian fitting to line intensities and widths that appear in columns (7), (8), and (9), respectively. Emission spectra corresponding to Table 1 data are shown in Figure 2 with emission features at LSR velocities

of  $+64$  and  $+82 \text{ km s}^{-1}$  which are characteristic of two clouds that lie superimposed along the same line of sight (see Fig. 7 of Mehringer & Menten [1997] and Fig. 2 of Hollis [2006]). The cyanoformaldehyde total beam-averaged column densities ( $N_T$ ) for the two LSR components were computed following the formalism employing cgs units (cf. Table 1 parameters) outlined in Hollis et al. (2000) for a spectral feature found in emission with a single-element radio telescope:

$$N_T = \frac{Qe^{E_u/kT_{\text{ex}}}}{(8\pi^3/3k)\nu S\mu^2} \frac{(1/2)\sqrt{\pi/\ln 2}(\Delta T_A^* \Delta V/\eta_B)}{1 - (e^{h\nu/kT_{\text{ex}}} - 1)/(e^{h\nu/kT_{\text{bg}}} - 1)}. \quad (1)$$

In equation (1), the line is assumed to be Gaussian;  $\nu$  is the transition frequency (col. [2]);  $S$  is the transition line strength (col. [3]);  $E_u$  is the upper rotational energy level which can be derived from columns (2) and (4) in Table 1;  $\eta_B$  is the telescope beam efficiency (col. [6]);  $\Delta T_A^*$  is the fitted peak line temperature (col. [8]);  $\Delta V$  is the fitted FWHM line width (col. [9]);  $T_{\text{bg}} \sim 2.7 \text{ K}$  is the cosmic background temperature;  $Q = 4.25T_{\text{ex}}^{3/2}$  is the partition function (see Gordy & Cook [1984, p. 58] for a more detailed formulation); and the electric dipole moment is  $\mu = \mu_b$  for the  $b$ -type transitions in Table 1, which we estimated as follows: From ab initio calculations, the total dipole moment estimates for CNCHO are  $\mu_T = 2.75 \text{ D}$  (Goddard 1986) and  $\mu_T = 2.80 \text{ D}$  (Császár 1989). Ab initio values of the total dipole moment should be scaled to agree with experimental values; hence, for CNCHO a scale factor of 89.6% was used based on ab initio calculations of the dipole moment for propynal (Goddard 1986) and the experimental determination for propynal (Brown & Godfrey 1984). Further, the  $\mu_a$ -to- $\mu_b$  dipole moment component ratio of 0.63 obtained from relative intensity measurements published in Bogey et al. (1995) was used in the expression  $(0.896\mu_T)^2 = \mu_a^2 + \mu_b^2$  which yields  $\mu_a \sim 1.3 \text{ D}$  and  $\mu_b \sim 2.1 \text{ D}$ . A CNCHO excitation temperature  $T_{\text{ex}} \sim 8 \text{ K}$  was assumed, and will be justified in the next section. Using the aforementioned parameter values, equation (1) yields the beam-averaged column densities that appear in column (10) of Table 1 for each emission velocity component of each CNCHO transition. In total, the CNCHO column density ranges from 1 to  $17 \times 10^{14} \text{ cm}^{-2}$ . For a molecular  $\text{H}_2$  column density of  $1.6 \times 10^{23} \text{ cm}^{-2}$  (derived from the Martin et al. [2004] data), the CNCHO fractional abundance ranges from 0.7 to  $11 \times$

TABLE 1  
SUMMARY OF CYANOFORMALDEHYDE TRANSITIONS SOUGHT TOWARD SGR B2(N)

Transition $J'(K_-, K_+) - J''(K_-, K_+)$ (1)	Frequency <sup>a</sup> (MHz) (2)	$S$ (3)	$E_l$ ( $\text{cm}^{-1}$ ) (4)	$\theta_B$ (arcsec) (5)	$\eta_B$ (6)	$V_{\text{LSR}}$ ( $\text{km s}^{-1}$ ) (7)	$T_A^b$ (mK) (8)	$\Delta V^b$ ( $\text{km s}^{-1}$ ) (9)	$N_T^c$ ( $\times 10^{14} \text{ cm}^{-2}$ ) (10)
5(1, 5)–6(0, 6) .....	2078.068(11)	2.5987	6.768	350	0.97	+64	-119(8)	25.2(13)	...
7(0, 7)–6(1, 6) .....	8574.116(12)	3.1521	8.736	86	0.95	+64	97.0(1)	15.9(2)	17.40(25)
						+82	46.9(2)	9.4(3)	4.96(18)
4(1, 4)–5(0, 5) .....	12580.250(10)	2.0593	4.835	59	0.93	<sup>d</sup>			
8(0, 8)–7(1, 7) .....	19367.997(13)	3.7215	10.951	38	0.88	+64	33.9(1)	13.5(4)	3.21(11)
						+82	28.3(1)	13.9(4)	2.76(9)
3(1, 3)–4(0, 4) .....	22925.235(9)	1.5318	3.224	32	0.84	<sup>d</sup>			
9(0, 9)–8(1, 8) .....	30294.182(14)	4.3089	13.483	24	0.76	+64	22.8(13)	13.4(7)	2.24(26)
						+82	19.7(12)	13.4(7)	1.94(22)
2(1, 2)–3(0, 3) .....	33106.952(9)	1.0141	1.934	22	0.72	+64	<30	...	...
10(0, 10)–9(1, 9) .....	41342.225(15)	4.9159	16.330	18	0.62	+64	12.5(13)	20.6(16)	2.58(47)
						+82	6.1(16)	17.0(27)	1.04(44)

<sup>a</sup> Rest frequencies and molecular line parameters were calculated from spectroscopic data in Bogey et al. (1988, 1995). Uncertainties in parentheses refer to the least significant digit and are  $2\sigma$  values (Taylor & Kuyatt 1994).

<sup>b</sup> Gaussian fit values with  $1\sigma$  uncertainties; upper limit is  $3\sigma$ .

<sup>c</sup>  $T_{\text{ex}} = 8 \text{ K}$  for all calculations with  $1\sigma$  uncertainties that reflect only the uncertainties in cols. (8) and (9).

<sup>d</sup> The 12.6 GHz transition is coincident with strong RFI features and the 22.9 GHz transition is coincident with a prominent  $\text{NH}_3$  line. Thus, these features were not detected.

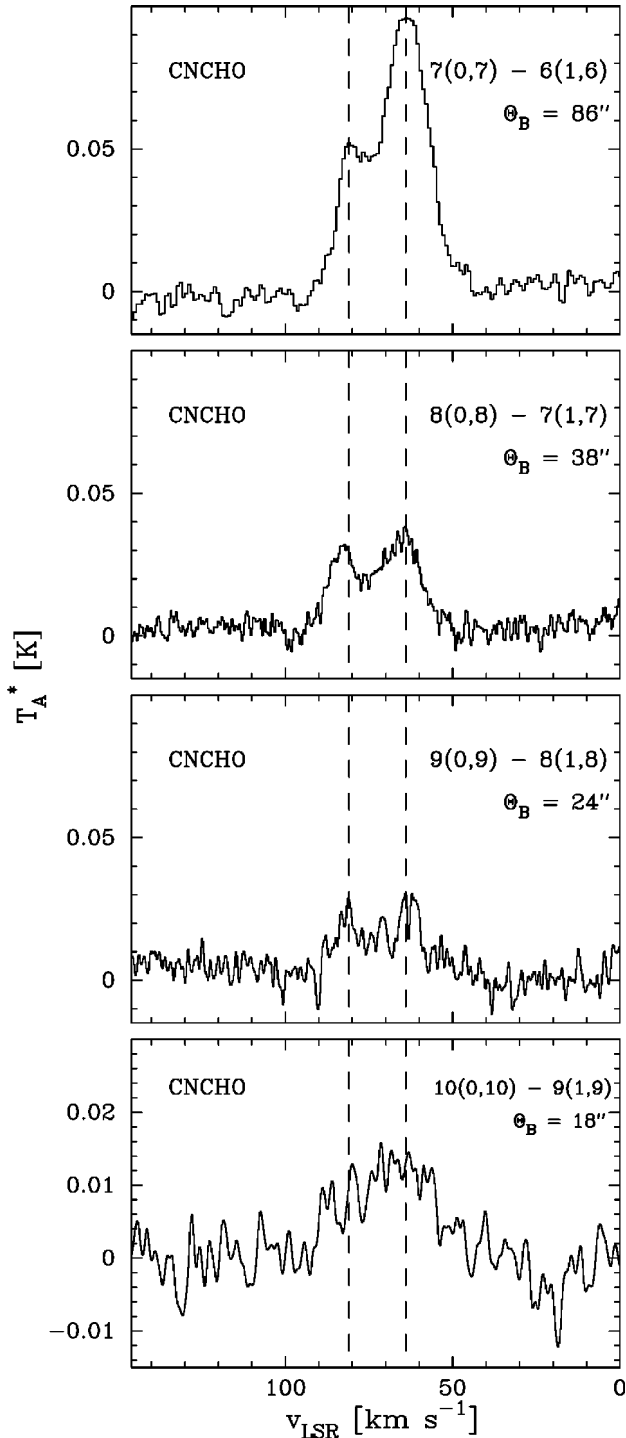


FIG. 2.—Cyanoformaldehyde emission spectra toward Sgr B2(N). Transition quantum numbers and beam sizes are shown in each panel. Each abscissa is LSR velocity calculated for the transition rest frequency (see Table 1) at an assumed LSR source velocity of  $+64 \text{ km s}^{-1}$ . Dashed lines show LSR velocities at  $+64$  and  $+82 \text{ km s}^{-1}$ . Data in the last two panels were Hanning smoothed for display purposes.

$10^{-9}$ . The relative abundance ratio of CNCHO with respect to other detected interstellar aldehydes is discussed in § 3.

### 3. DISCUSSION

Recent observations with the Berkeley Illinois Maryland Association (BIMA) Array and the GBT toward Sgr B2(N-LMH) and the Giant Metrewave Radio Telescope (GMRT) toward Sgr B2

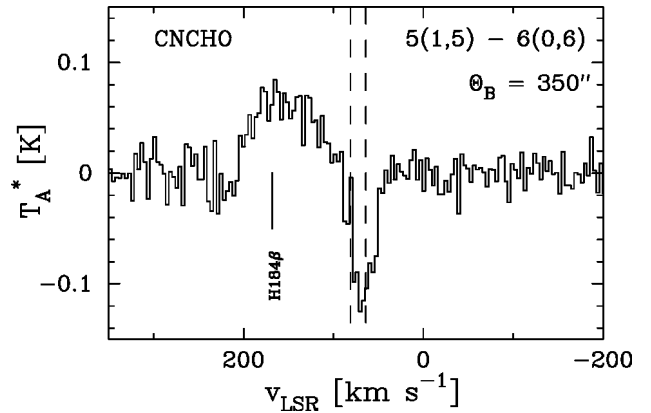


FIG. 3.—Cyanoformaldehyde absorption spectrum toward Sgr B2(N). Figure annotations and labels are similar to Fig. 2. Cyanide line lies close to H184 $\beta$ .

indicate that large aldehyde molecules such as glycolaldehyde ( $\text{CH}_2\text{OHCHO}$ ; Hollis et al. 2001), acetaldehyde ( $\text{CH}_3\text{CHO}$ ; Chenguang & Kanekar 2003), propenal ( $\text{CH}_2\text{CHCHO}$ ; Hollis et al. 2004b), and propanal ( $\text{CH}_3\text{CH}_2\text{CHO}$ ; Hollis et al. 2004b) are spatially extended. These molecules survive in the cold halo regions, undergoing transitions between low-energy levels that tend to occur in the frequency range of 1 to 48 GHz. For example, the GBT detected four  $\text{CH}_2\text{OHCHO}$  transitions in the halo region surrounding the LMH hot core where all transitions had energies less than 6.5 K. The subsequent analysis of these four rotational transitions yielded a  $\text{CH}_2\text{OHCHO}$  excitation temperature of  $\sim 8 \text{ K}$  (Hollis et al. 2004a) which is probably characteristic of the cold halo region surrounding the LMH.

The CNCHO column density measurements in Table 1, column (10), clearly suggest an extended source of CNCHO that is most likely not uniformly distributed. For example, the  $+64 \text{ km s}^{-1}$  LSR component for the  $7(0, 7)$ – $6(1, 6)$  transition yields a beam-averaged column density  $\sim 5$  times that obtained from the  $8(0, 8)$ – $7(1, 7)$  transition. Similarly, the  $+82 \text{ km s}^{-1}$  LSR component of the  $7(0, 7)$ – $6(1, 6)$  transition yields a beam-averaged column density  $\sim 2$  times that obtained from the  $8(0, 8)$ – $7(1, 7)$  transition. It is likely that the beam area of the  $7(0, 7)$ – $6(1, 6)$  transition, which is  $\sim 5$  times the beam area of the  $8(0, 8)$ – $7(1, 7)$  transition, is detecting additional emission, particularly from Sgr B2(M), which is  $\sim 45'$  south of the Sgr B2(N-LMH) pointing position. Moreover, when sources are larger than the beam size, the telescope error beam can contribute significantly to the observed emission and the source-beam coupling can be quite complex (e.g., Gordon et al. 1992). As shown in Figure 3, the  $5(1, 5)$ – $6(0, 6)$  transition was observed in absorption with a GBT beam width of  $\sim 350'$ , thus observationally demonstrating that CNCHO has a widespread spatial distribution.

Other cyanoformaldehyde transitions in the P branch sequence that are lower in energy and lower in transition line strength but comparable in frequency to the four detected transitions are the  $4(1, 4)$ – $5(0, 5)$  at 12.6 GHz, the  $3(1, 3)$ – $4(0, 4)$  at 22.9 GHz, and the  $2(1, 2)$ – $3(0, 3)$  at 33.1 GHz (Table 1). The  $4(1, 4)$ – $5(0, 5)$  and the  $3(1, 3)$ – $4(0, 4)$  transitions are coincident with strong RFI and a prominent  $\text{NH}_3$  line, respectively, and cannot be observed. Observations were attempted for the  $2(1, 2)$ – $3(0, 3)$  transition but no significant emission (see Table 1) was detected presumably because this P-branch transition has a low transition line strength and transitions between lower energy levels are susceptible to the competing effects of absorption.

From transition line strength and electric dipole moment arguments, the most favorable interstellar CNCHO transitions are *b*-type transitions of the *P*, *Q*, and *R* branches in which *K<sub>a</sub>* changes from

0 to 1 or 1 to 0. The four such *P*-branch transitions observed in emission toward Sgr B2(N) are expected to be less intense than those favorable *R*-branch transitions that occur within the range of 80–160 GHz. Presumably some of these favorable *R*-branch transitions were the target of CNCHO searches at higher frequencies that did not result in positive detections. For example, the most recently reported search attempt toward Sgr B2(N) utilized the Arizona Radio Observatory (ARO) 12 m telescope operating in the range of 70–170 GHz (Woolf 2006); however, no observational details were given other than a reported nondetection of CNCHO. The only other previously reported searches were toward Sgr B2(OH) and Orion Irc2 with the Swedish ESO Submillimetre Telescope (SEST) 15 m telescope operating in the range of 80–115 GHz, and the Institut de Radioastronomie Millimétrique (IRAM) 30 m telescope operating in the range of 96–217 GHz (Gerin et al. 1989). These searches achieved only modest noise limits.

The column density of CNCHO can be compared with column densities of other widespread aldehyde species toward the Sgr B2(N) region to arrive at estimates of relative abundances. For example, it has been established that glycolaldehyde in the extended region surrounding Sgr B2(N) is characterized by an excitation temperature of  $\sim 8$  K (see, e.g., Hollis et al. 2004a). As determined from equation (1) in § 2, the total CNCHO column density range is  $(1\text{--}17) \times 10^{14} \text{ cm}^{-2}$  for a  $T_{\text{ex}} = 8$  K. This range is similar to the column density determined for  $\text{CH}_2\text{OHCHO}$  of  $3.5 \times 10^{14} \text{ cm}^{-2}$  from Hollis et al. (2004a). The relative abundance of CNCHO is 0.2–0.5 compared to the column density of formamide ( $\text{NH}_2\text{CHO}$ ) of  $(6\text{--}61) \times 10^{14} \text{ cm}^{-2}$  from Hollis et al. (2006). Thus, given the abundance uncertainty ranges, the total column densities of CNCHO,  $\text{CH}_2\text{OHCHO}$ , and  $\text{NH}_2\text{CHO}$  are all similar when measured with the GBT. What we have also assumed is that the temperature and especially the density is high enough to thermalize and populate all the transitions from centimeter to millimeter wavelengths. However, even though the lower state energies and line strengths of the millimeter lines are comparable to the centimeter lines, the Einstein *A* coefficients of the millimeter lines are much larger than the centimeter transitions, which may explain the lack of detection of CNCHO at millimeter wavelengths.

Current theoretical chemistry models do not reproduce the relative abundance ratios of large aldehydes detected with the GBT (Quan & Herbst 2007), so there is no accepted formation route to the synthesis of CNCHO in interstellar environments. Given its extended, nonuniform spatial distribution and low temperature, the reaction that produces CNCHO is likely fast and involves abundant reactants. We posit that cyanoformaldehyde could be formed from the reaction of the cyanide radical and neutral formaldehyde since both are known to have widespread spatial distributions and relatively high abundances in

interstellar clouds (e.g., Zuckerman & Palmer 1974; Churchwell 1980):



Radical-neutral reactions often can be barrierless and exothermic (e.g., Balucani et al. 2002). In equation (2) CNCHO would form from a substitution of the CN radical for one of the H in  $\text{H}_2\text{CO}$ . Since laboratory work found CNCHO is highly reactive with  $\text{H}_2\text{O}$  (Lewis-Bevin et al. 1992), gas-phase reactions of CNCHO with  $\text{H}_2\text{O}$  may account for its destruction in interstellar environments. Assuming that the formation of CNCHO is dominated by the reaction of CN with  $\text{H}_2\text{CO}$  with rate  $k_1$ , and that its destruction is due to the reaction with  $\text{H}_2\text{O}$  with rate  $k_2$ , the relative CNCHO abundance ratio can be determined as  $X(\text{CNCHO}) \sim k_1 \cdot X(\text{CN}) \cdot X(\text{H}_2\text{CO}) / k_2 \cdot X(\text{H}_2\text{O})$ ; with  $X(\text{CN}) \sim X(\text{H}_2\text{CO}) \sim 2 \times 10^{-8}$ ,  $X(\text{H}_2\text{O}) \sim 1 \times 10^{-7}$ , and  $k_1 \sim k_2$ ,  $X(\text{CNCHO}) \sim 4 \times 10^{-9}$ , which falls right in the observed range. Similarly, other interstellar molecules could be related to formaldehyde through substitution of a radical for one of its H atoms. For example, the formation of formic acid ( $\text{HCOOH}$ ), formamide ( $\text{NH}_2\text{CHO}$ ), propynal ( $\text{HC}_2\text{CHO}$ ), and acetaldehyde ( $\text{CH}_3\text{CHO}$ ) would employ the known interstellar radicals OH,  $\text{NH}_2$ ,  $\text{C}_2\text{H}$ , and  $\text{CH}_3$ , respectively. Furthermore, it is possible that given the highly reactive nature of CNCHO, it could be part of a larger chemical reaction network that can lead to the formation of more complex organic species in astronomical environments.

In summary, we have detected cyanoformaldehyde (CNCHO), a new interstellar molecule, by observing five low-frequency *P*-branch rotational transitions with the GBT toward Sgr B2(N). Since cyanoformaldehyde has aldehyde characteristics, we argue that this species is spatially widespread in a nonuniform distribution, and cold like many other aldehydes in the halo region of Sgr B2(N). It is also possible that in addition to the emission from Sgr B2(N), there could be a significant contribution of CNCHO emission from Sgr B2(M) and possibly Sgr B2(S), which may account for the widespread distribution. These conditions, in addition to the large Einstein *A* coefficients, may account for unsuccessful searches for cyanoformaldehyde by other investigators probing for higher frequency *Q*- and *R*-branch transitions. Therefore, while our conclusions that CNCHO has a low excitation temperature and an extended spatial distribution are consistent with the data presented, it is clear more observations are needed to determine the true spatial distribution and excitation conditions of this new molecule. Finally, we suggest that cyanoformaldehyde is likely formed by a neutral-radical reaction of formaldehyde ( $\text{H}_2\text{CO}$ ) and the cyanide (CN) radical since neutral-radical reactions often proceed exothermically without any activation barrier and these parent species are also found to have widespread spatial scales in interstellar clouds.

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